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MEMORANDUM FOR PR (Contractor/In-House Publication)

FROM: PROI (TI) (STINFO)

18 Apr 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2000-075**
Vij, V., Boatz, J.A., Tham, F., Vij, A., and Christe, K.O., "On the Lewis Acidity of LiF" (Abstract)

16th International Symposium of Fluorine Chemistry
(Durham, UK, 23 Jul 00) (Submission Deadline: 18 Apr 2000)

(Statement A)

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PHILIP A. KESSEL Date _____
Technical Advisor
Propulsion Science and Advanced Concepts Division

ON THE LEWIS ACIDITY OF LiF

V. Vij, J. A. Boatz, F. Tham, A. Vij and K. O. Christe*

Air Force Research Laboratory, Edwards Air Force Base CA, USA, Loker Hydrocarbon Research Institute, University of Southern California, Los Angeles, CA, USA, and Department of Chemistry, University of California, Riverside, CA, USA

Based on the recently developed pF^- Lewis acidity scale,¹ free gaseous LiF is a surprisingly strong Lewis acid, comparable to SiF_4 . It was therefore of interest to study whether a strong Lewis base, such as CsF, could transfer a fluoride ion to LiF with formation of a LiF_2^- anion. Theoretical calculations were carried out for LiF_2^- and show that free gaseous LiF_2^- is a linear, vibrationally stable species. Furthermore, the phase-diagram of the LiF/CsF system shows a eutectic at a 1:1 mole ratio that gives a distinct X-ray powder diffraction pattern.² We have prepared this eutectic by fusion of a 1:1 mixture of LiF and CsF in a platinum crucible. Single crystals were obtained by slow cooling of the melt in a dry nitrogen stream. The resulting product was characterized by vibrational spectroscopy, and its crystal structure was determined. It is shown that $CsLiF_2$ does not contain isolated LiF_2^- anions, but exhibits an interesting three-dimensional network of alternating tetra-coordinated LiF_4 and octa-coordinated CsF_8 units.

1. K. O. Christe, D. A. Dixon, D. McLemore, W. W. Wilson, J. A. Sheehy and J. A. Boatz, *J. Fluorine Chem.*, 2000, **101**, 151.
2. D. L. Deadmore and J. S. Machin, *J. Phys. Chem.*, 1960, **64**, 824.